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AquiMod User Manual (v1.0)

Environmental Modelling Programme

Open Report OR/14/007

BRITISH GEOLOGICAL SURVEY

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Summary

This user manual describes AquiMod, a simple lumped groundwater level simulation model. It details the mathematical structure of the model and provides some guidance for configuring and running the software on a Windows PC. All examples shown were undertaken on a computer running Windows 7, and as such, some of the steps may differ when using a different version of the Windows operating system.

1 Overview

AquiMod is a lumped parameter computer model that has been developed to simulate groundwater level time-series at observation boreholes in aquifers by linking simple hydrological algorithms that model soil drainage, the transfer of water through the unsaturated zone and groundwater flow. It runs on a Windows PC through the command prompt and is configured using a series of text files. The simple structure of AquiMod makes it easy to use in comparison to more complex physically-based distributed models, and therefore should be accessible to those users who are new to the field of groundwater/hydrological modelling. It uses conceptual modelling approaches that are in line with general hydrological process understanding and has been used in the past to teach hydrological modelling concepts to Earth Science undergraduates. The main features of the AquiMod software include:

- Fast simulation of groundwater level time-series
- Flexible time-stepping
- Monte Carlo parameter sampling
- Modular structure with multiple process representations
- Choice of objective functions to evaluate model efficiency

1.1 INTENDED USE

AquiMod can be applied to any groundwater catchment around an observation borehole with observed groundwater level time-series data. It can be calibrated against these data and used to provide information on the behaviour of groundwater levels beyond observational records. The model has been used in this way for a number of applications, including reconstructing groundwater level records, long term projections of groundwater levels under climate change and forecasting groundwater levels into the near future using meteorological forecasts. Of course, this list of applications is not absolute and users are encouraged to experiment with the software. However, it is important to consider the limitations of the AquiMod when deciding if it is suitable for your intended use. Please refer to a summary of these limitations in (Table 1.1).

Table 1.1 Considerations and potential limitations when applying AquiMod for groundwater level simulation.

Consideration	Limitation
Lumped model structure	AquiMod lumps the catchment area into a single response unit which is characterised by a groundwater level borehole hydrograph. It treats each input variable (e.g. soil type and rainfall) and output variable (e.g. groundwater level) as spatially uniform over your chosen study area and therefore cannot provide information on spatial heterogeneity within a given catchment area.
Time-series data	AquiMod needs observed groundwater level time-series to evaluate the model against and corresponding rainfall and potential evapotranspiration (PET) data to drive the model.
Model boundary	AquiMod assumes that the groundwater catchment receives recharge from rainfall only, i.e. it does not account for other sources of recharge such as lateral groundwater flows across the catchment boundary.

1.2 GENERALISED STRUCTURE

AquiMod consists of three modules (Figure 1.1). The first is a soil water balance module that partitions rainfall between evapotranspiration, runoff and soil drainage. This module simulates the water balance of the root zone, therefore soil drainage is defined as the water that percolates past the root zone and is no longer available for evapotranspiration. Drainage from the soil is then attenuated through an unsaturated zone module which represents percolation to the groundwater table as recharge. This recharge is input to the saturated zone module that simulates aquifer storage and subsequent discharge. It is the saturated zone module that calculates the groundwater level time-series.

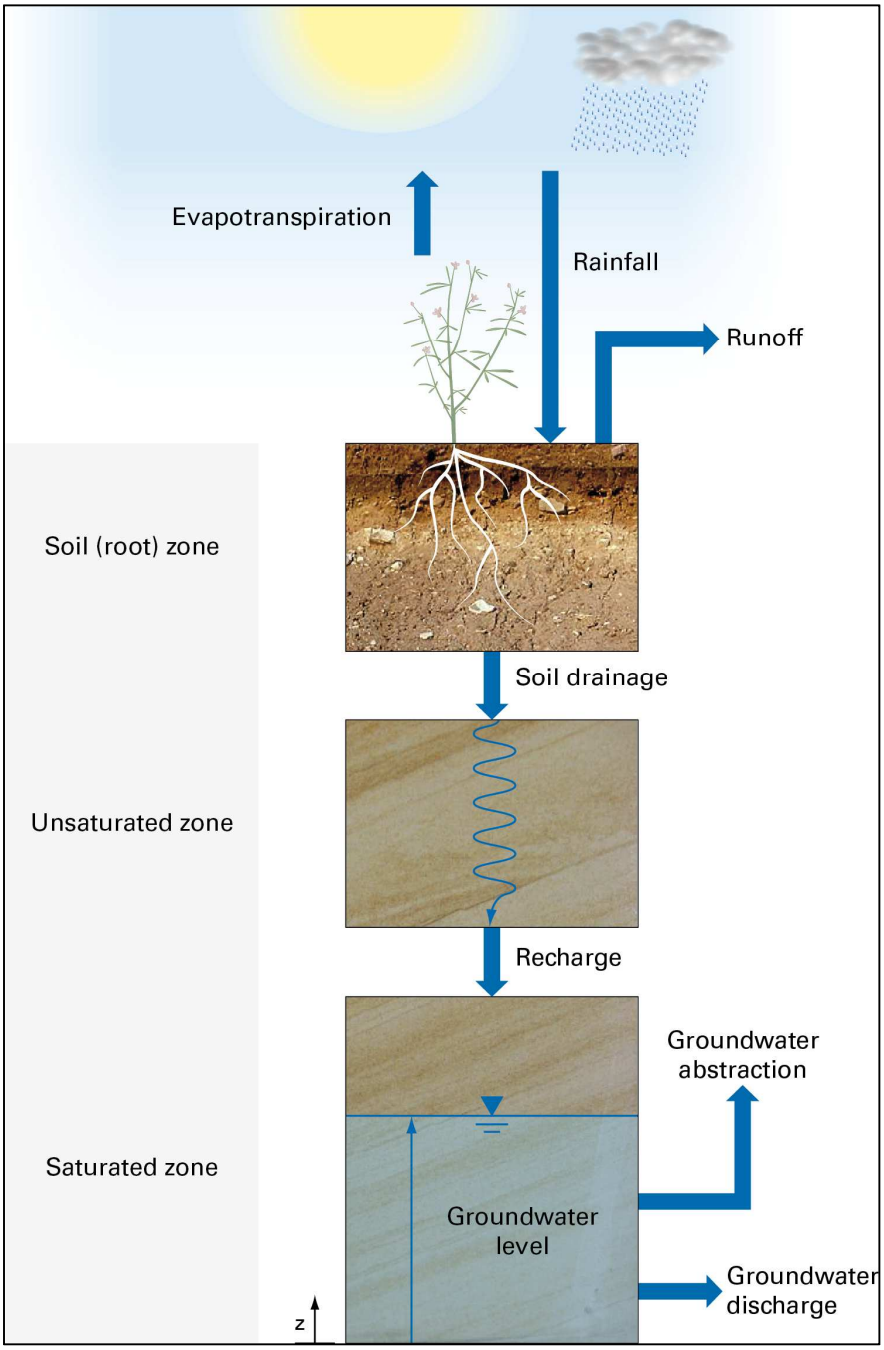

Figure 1.1 Generalised structure of AquiMod.

2 Getting started

2.1 INSTALLATION

Before starting, you'll need to download the AquiMod software, which is available directly from the British Geological Survey website at:

http://www.bgs.ac.uk/research/environmentalmodelling/aquimod.

The download package includes the AquiMod executable, located within the AquiMod folder, an example model build which is located within the CHexample folder, and a series of template files located in the Template folder which can be used when constructing a new model. If this is the first time you've used this software, we recommend that you copy all of the folders to your hard disk[1] as some of the files are required for the Tutorials section. Next, you must add the AquiMod folder to the Windows Path environment variable (this makes it easier to run AquiMod from the command line). For this, do the following:

- From the Start menu right-click **Computer** and select **Properties** from the dropdown menu.
- Select **Advanced System Settings** in the left column. This will open the **System Properties** windows (Figure 2.1).
- Under the **Advanced** tab, click the **Environment Variables** button.

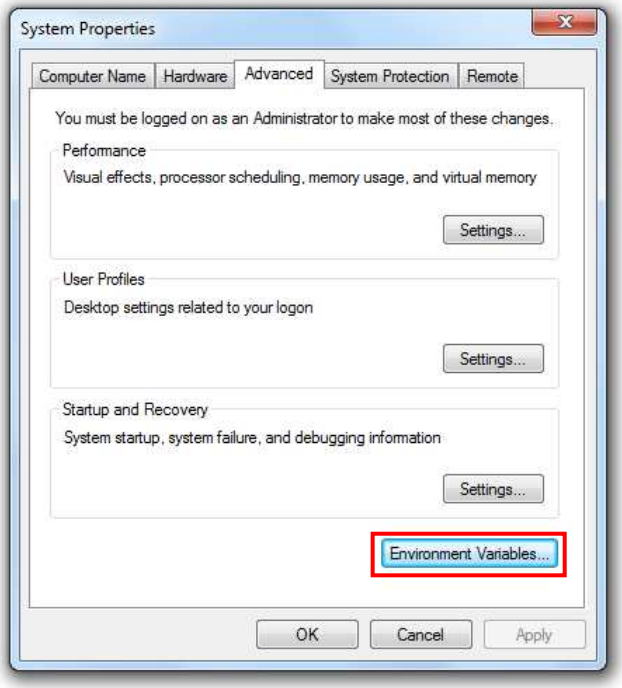

Figure 2.1 System properties window.

[1] IMPORTANT: The path address for the CHexample folder must contain no whitespace.

- Under the **System Variables** header find the **Path** variable and click **Edit** (Figure 2.2).

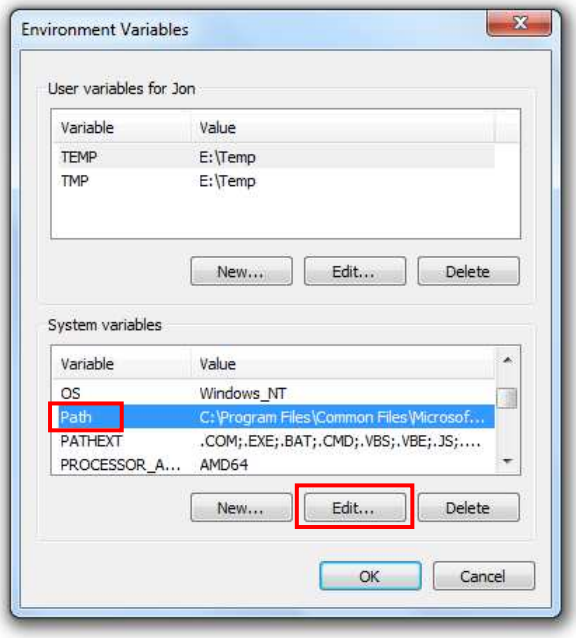

Figure 2.2 Environment Variables window.

- At the end of the **Path Variable** value line, insert a semicolon followed by the address of the AquiMod folder. In the example shown in Figure 2.3 this folder was copied directly to the C-drive.

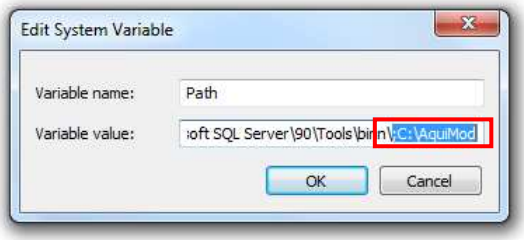

Figure 2.3 Edit System Variable window.

AquiMod is now ready to use.

2.2 RUNNING AQUIMOD

The AquiMod executable is run using the Windows command prompt which can be accessed by typing ‘cmd’ into the search bar of the Start menu and hitting the return key. Once the command prompt has loaded, AquiMod can be run by typing ‘aquimod’ followed by the directory address of the model files separated by a space. The CHexample folder contains an example model build that is ready to run. In the command prompt **type aquimod followed by the location of the CHexample folder** as shown in Figure 2.4.

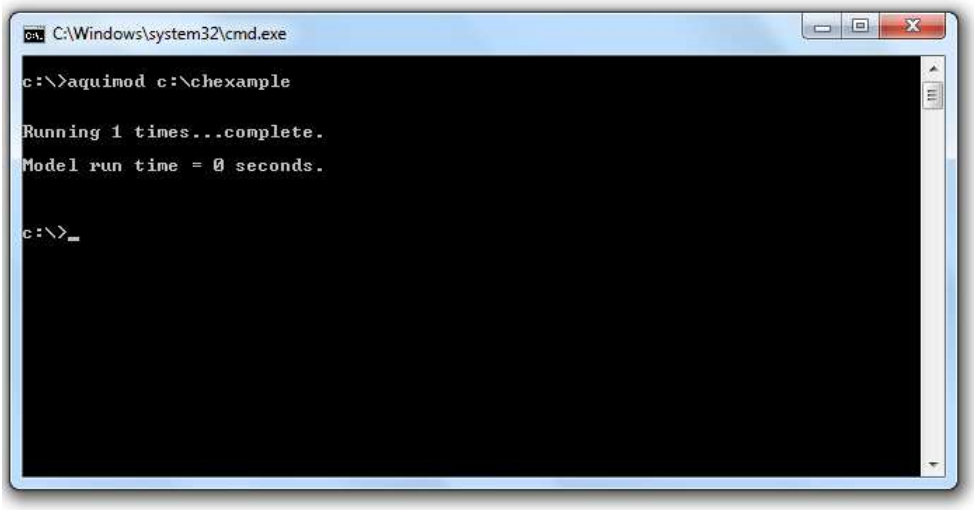

Figure 2.4 Running AquiMod through the command prompt.

Notice that AquiMod provides output messages to indicate that the model run has completed. If you **navigate to the Output folder**, you’ll notice a series of files with the ‘.out’ extension. These are output files produced by AquiMod. They are text files that can be viewed in your text editor.

3 Modules

AquiMod has three modules that represent the soil, unsaturated and saturated zone hydrology. Each module has been designed so that it can incorporate a number of possible structures (components), each based on a different conceptual representation of the process being considered, but all of which adhere to the same generalised structure outlined in section 1.2. Each component uses one or more parameters which can be modified to change the behaviour of the model. These parameters and the mathematical algorithms that AquiMod employs are described below. Please note also, that all component parameters and recommended calibration ranges are listed in Appendix 1.

3.1 SOIL ZONE MODULE

Currently there is only one soil zone component available in the AquiMod software (Table 3.1).

Table 3.1 Summary of soil zone module components.

ID	Name	Description
1	FAO	Drainage from the base of the soil zone is calculated using a soil water balance method based on a simplification of the algorithm developed by the UN Food and Agricultural Organisation (Allen et al., 1998).

3.1.1 FAO

This component simulates soil moisture as a function of vegetation and soil properties. The soil column is conceptualised as a bucket with a maximum volume of water available to plants after the soil has drained to its field capacity (Figure 3.1a). This is termed the *total available water* (TAW) which is calculated as:

$$TAW = Z_r(FC - WP) \quad (1)$$

where Z_r is the estimated *maximum root depth* [L] of the vegetation, and FC and WP are the *soil field capacity* and *wilting point*, respectively.

As the soil moisture content decreases, it becomes more difficult for vegetation to extract moisture from the soil matrix. The proportion of TAW that can easily be extracted before this point is reached is conceptualised as *readily available water* (RAW), which is calculated as:

$$RAW = p \cdot TAW \quad (2)$$

where p is the *depletion factor* of the vegetation.

The water balance of the soil zone is a function of the rainfall input and evaporative flux from the soil and can be written as:

$$\Delta SMD = AET - PPTN \quad (3)$$

where SMD is the *soil moisture deficit* [L], PPTN is the total *precipitation* input [L] and AET is the *actual evapotranspiration* [L], which is calculated as a function of *potential evapotranspiration* (PET) [L] and the SMD (Figure 3.1b):

$$\begin{aligned} AET &= PET\left[\frac{TAW - SMD^*}{TAW - RAW}\right]^{0.2} && SMD^* > RAW \\ AET &= PET && SMD^* \leq RAW \\ AET &= 0 && SMD^* \geq TAW \end{aligned} \qquad (4)$$

When the soil zone becomes saturated any rainfall in excess of the evaporative demand of the vegetation becomes *excess water* (EXW). This excess water is then split between soil drainage and *surface runoff*. The proportion of the excess water (EXW) that drains to the unsaturated zone is:

$$SD = BFI \cdot EXW \qquad (5)$$

where SD is the soil drainage and BFI is the *baseflow index*, which defines the average proportion of stream flow that a river receives from groundwater discharge. Surface runoff is then calculated as the remainder of the excess water.

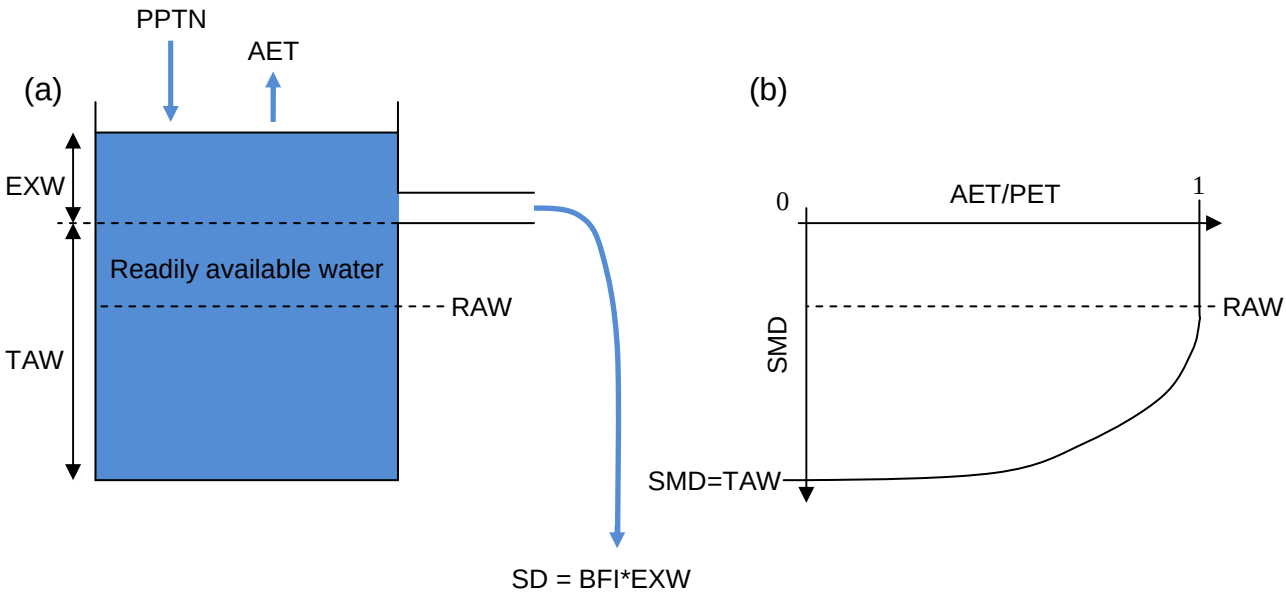

Figure 3.1 (a) FAO soil zone component conceptualised as a bucket with a finite capacity and (b) the change in ratio of AET to PET with SMD as described by equation 4.

3.2 UNSATURATED ZONE MODULE

Currently there is only one unsaturated zone component available in the AquiMod software (Table 3.2).

Table 3.2 Summary of unsaturated zone module components.

ID	Name	Description
1	Weibull	Drainage from the soil is attenuated through the unsaturated zone using a Weibull distribution transfer function.

3.2.1 Weibull

Recharge is distributed over a number of time-steps, n, and the proportion of soil drainage for each time-step is calculated using a two-parameter Weibull probability density function:

$$f(x;\lambda,k) = \begin{cases} \frac{k}{\lambda}\left(\frac{x}{\lambda}\right)^{k-1} e^{-(x/\lambda)^k} & x \geq 0 \\ 0 & x < 0 \end{cases} \quad (6)$$

where k > 0 is the shape parameter and λ > 0 is the scale parameter of the distribution. The λ parameter primarily controls the location of the peak in the probability density function while k controls the density of the function around the peak (Figure 3.2). The resulting distribution is scaled such that the discrete integral of f is equal to unity and consequently the recharge for each time-step (R_t) is spread over the selected number of time-steps, n:

$$R_t = \alpha \sum_{x=1}^{n} f(x) \cdot SD_{t-x+1} \quad (7)$$

where α is the scaling parameter. The Weibull function can represent exponentially increasing, exponentially decreasing, and positively and negatively skewed distributions. It is used because it allows the exploration of different distributions, whilst being smooth, which is considered to be more physically justifiable than randomly selected monthly weights.

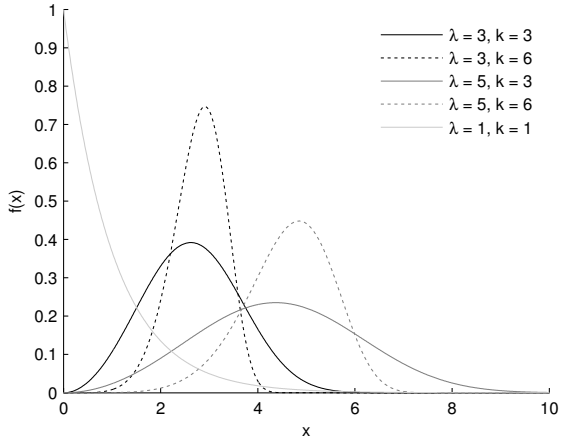

Figure 3.2 Probability distribution function of the Weibull distribution using different λ and k combinations.

3.3 SATURATED ZONE MODULE

There are currently five different saturated zone components available in the AquiMod software as summarised in Table 3.3.

Table 3.3 Summary of saturated zone module components.

ID	Name	Description
1	Q3K3S1	A three-layer aquifer representation, each of variable thickness and permeability.
2	Q2K2S1	A two-layer aquifer representation, each of variable thickness and permeability.
3	Q1K1S1	A single layer aquifer representation.
4	Q1T1S1	A confined aquifer representation with a fixed transmissivity.
5	VKD	An aquifer with a 'cocktail glass' representation of the change in hydraulic conductivity with depth.

3.3.1 Q3K3S1

This component represents flow in the saturated zone by a rectangular block of aquifer with dimensions Δx and Δy denoting its length and width [L] respectively. A mass balance calculation is performed at each time-step to calculate the new groundwater head:

$$R\Delta x\Delta y - Q - A = S\Delta x\Delta y\frac{dh}{dt} \tag{8}$$

where R is recharge input [L T^{-1}], Q is the total groundwater discharge [L^3 T^{-1}], A [L^3 T^{-1}] is any additional abstraction, S is the storage coefficient (dimensionless), and dh is the change in groundwater head [L] over time, dt [T].

This component accommodates three layers of variable thickness and permeability (Figure 3.3). Each layer is independent and has its own discharge outlet. The deepest layer represents groundwater which flows out of the catchment via subsurface flow paths. The two upper outlets are lumped representations of surface discharge points in the catchment including rivers and springs. Both may flow intermittently if the groundwater head falls below the outlet elevation.

The total groundwater discharge is the sum of discharge from all layers in the saturated zone which is calculated using an equation of the form:

$$Q = \sum_{i=1}^{m} \frac{T_i \Delta y}{0.5\Delta x}\Delta h_i \tag{9}$$

where i is the layer number for m layers and Δh_i [L] is the difference between the groundwater head and the elevation of the aquifer outlet point. Importantly due to the explicit form of Equation 9 used, the groundwater head at the previous time-step, h^* [L] is used:

$$\Delta h_i = \begin{cases} h^* - z_i & h^* > z_i \\ 0 & h^* \leq z_i \end{cases} \tag{10}$$

where z_i is the outlet elevation. Transmissivity, T_i [L^2 T^{-1}] is a function of the hydraulic conductivity [L T^{-1}], k_i, and is calculated using the following piece-wise function:

$$T_i = \begin{cases} 0 & h^* \le z_i & i = (1 \dots m) \\ K_i(h^* - z_i) & z_i < h^* < z_{i+1} & i < m \\ K_i(z_{i+1} - z_i) & h^* \ge z_{i+1} & i < m \\ K_m(h^* - z_m) & h^* > z_m & i = m \end{cases} \quad (11)$$

Using this component, the hydraulic conductivity can be configured to increase or decrease with depth according to the user's preference. However, for some aquifers it may be preferable to have an increasing hydraulic conductivity with elevation. As such, an additional α parameter also exists for this component which can be switched to force this condition when using randomly sampled Monte Carlo parameter sets (See Appendix 1).

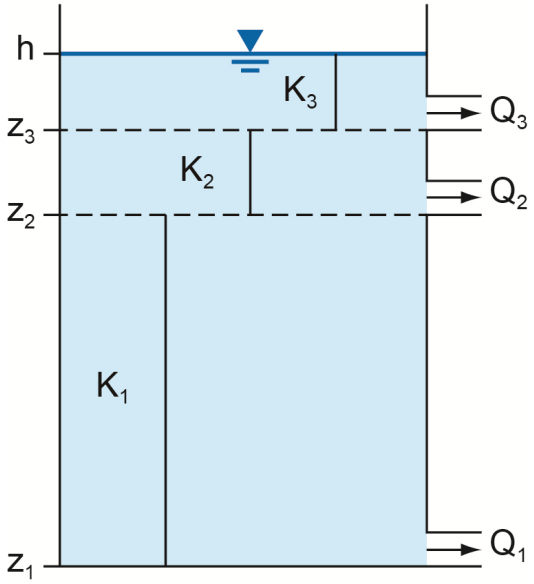

Figure 3.3 Q3K3S1 saturated zone component.

3.3.2 Q2K2S1

This component employs the same structure according to equations 8-11, however, here only two layers are defined. Each layer is independent and has its own discharge outlet (Figure 3.4). The deepest layer represents groundwater which flows out of the catchment via subsurface flow paths. The upper outlet is a lumped representation of surface discharge points in the catchment including rivers and springs. It may flow intermittently if the groundwater head falls below the outlet elevation. As with the Q3K3S1 component, the hydraulic conductivity can be forced to increase with elevation when using randomly sampled parameter sets by specifying the α parameter.

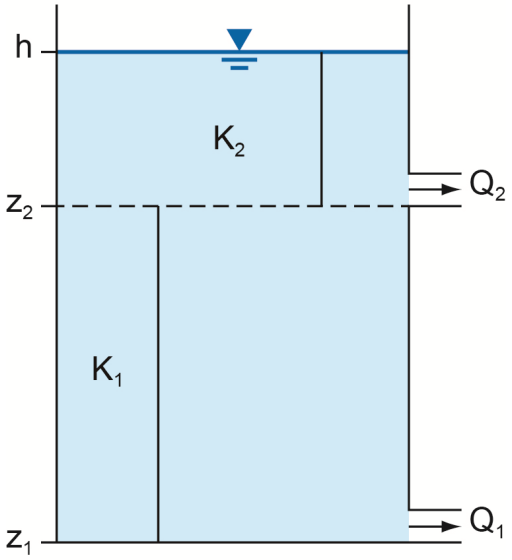

Figure 3.4 Q2K2S1 saturated zone component.

3.3.3 Q1K1S1

This component employs the same structure according to equations 8-11, however, here only one layer is defined with a single discharge outlet (Figure 3.5).

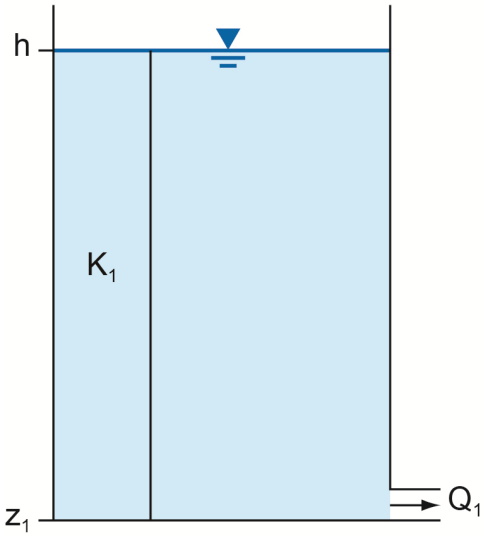

Figure 3.5 Q1K1S1 saturated zone component.

3.3.4 Q1T1S1

Like the Q1K1S1 saturated zone component, this component also employs a single outlet (Figure 3.6). However, the transmissivity is assumed to be fixed and independent of the hydraulic head, h. This is equivalent to a confined aquifer representation.

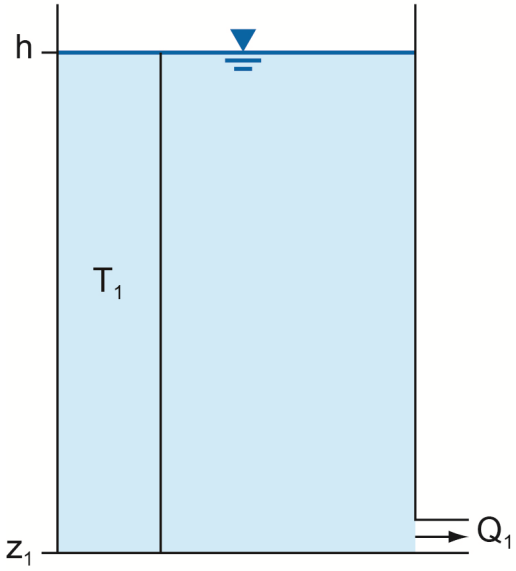

Figure 3.6 Q1T1S1 saturated zone component.

3.3.5 VKD

As an alternative to using specified layers and outlets, the user can also implement a variable conductivity with depth (VKD) profile. Here a 'cocktail glass' representation is can be employed which has two distinct sections (Figure 3.7). In the lower section, between the base of the aquifer, z_1 and the elevation of the point of inflection, z_p, the hydraulic conductivity is constant. In the upper section above z_p, the hydraulic conductivity increases linearly with elevation. Subsequently, the transmissivity is calculated as:

$$T = K_1(h^* - z_1) + 0.5 \cdot m\left(h^* - z_p\right)^2 \quad (12)$$

where K_1 is the hydraulic conductivity at the base of the aquifer and m is the gradient of the hydraulic conductivity profile above the point of inflection. The total discharge is then calculated as before:

$$Q = \frac{T\Delta y}{0.5\Delta x}(h^* - z_1) \quad (13)$$

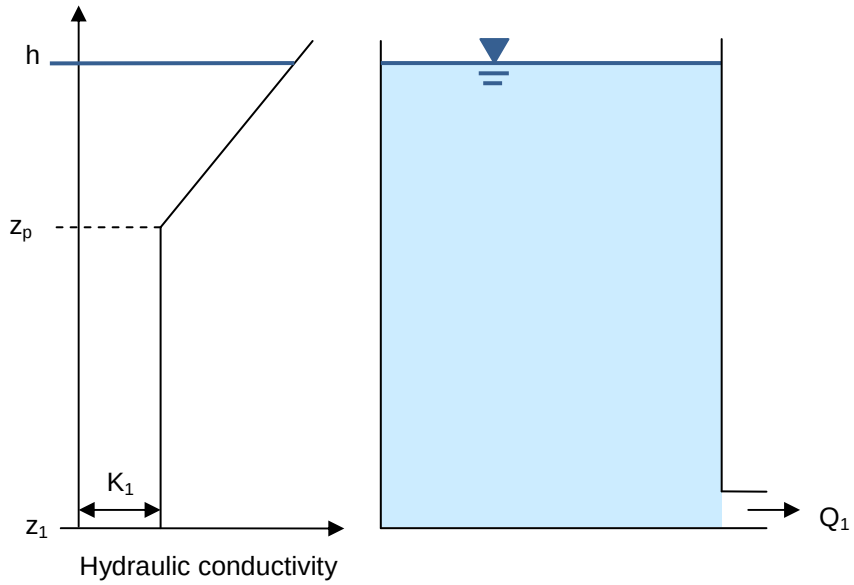

Figure 3.7 VKD saturated zone component.

4 Simulation modes

AquiMod has two different simulation modes, calibration and evaluation, which are described below.

4.1 CALIBRATION

The calibration mode is used to determine the most efficient model structures and parameter sets for the chosen application, i.e. those that produce groundwater level time-series that best replicate available observational data. In calibration mode, AquiMod has an in-built Monte Carlo parameter sampling algorithm that runs a specified model structure using multiple unique parameter sets (up to ~10^7) which are randomly sampled from a user-defined parameter space. For each parameter set, the model is run and a measure of simulation efficiency is calculated by comparing the simulated groundwater level time-series to available observed data. Three different objective functions can be used in AquiMod to determine model efficiency (Table 4.1).

Table 4.1 Objective functions available in AquiMod for a simulation sequence with n time-steps calculated using the observed (h_o) and modelled (h_m) groundwater levels.

ID	Name	Description
1	Nash-Sutcliffe Efficiency (NSE)	$NSE = 1 - \frac{\sum_{t=1}^{n}(h_o^t - h_m^t)^2}{\sum_{t=1}^{n}\left(h_o^t - \overline{h_o}\right)^2}$
2	Root Mean Squared Error (RMSE)	$RMSE = \sqrt{\sum_{t=1}^{n}(h_o^t - h_m^t)n^{-1}}$
3	Mean Absolute Percentage Error (MAPE)	$MAPE = \sum_{t=1}^{n}\left\lvert\frac{(h_o^t - h_m^t)}{h_o^t}\right\rvert n^{-1}$

4.2 EVALUATION

When using the evaluation mode, the user is required to specify one or more fixed parameter sets. AquiMod then determines the model efficiency for each of these and also generates time-series output files for each model component (e.g. groundwater level time-series for the saturated zone).

5 Model Files

This section provides more details about the model files that are used to configure AquiMod as well as the output files produced by the software. Most text editors are suitable for reading and editing AquiMod files, although it is advantageous to use an editor that displays line numbers as these are used in the file tables in this section. Examples include Notepad++ and PSPad, both of which are freely available to download from the internet.

5.1 GENERAL FILE AND FOLDER STRUCTURE

All of the information required to configure and run AquiMod is stored in a series of text files within a defined folder structure (Figure 5.1). The Observations.txt file contains all of the available observational data including rainfall, PET, groundwater level and abstraction rates. The Input.txt file allows the user to specify a number of options such as which module components and simulation mode they wish to use. The files stored in the Calibration and Evaluation folders are only used when AquiMod is set to run in these respective modes. They contain ranges or specific parameter values to be used by AquiMod when running in calibration and evaluation mode respectively. Finally, the Output folder is where all model outputs are generated.

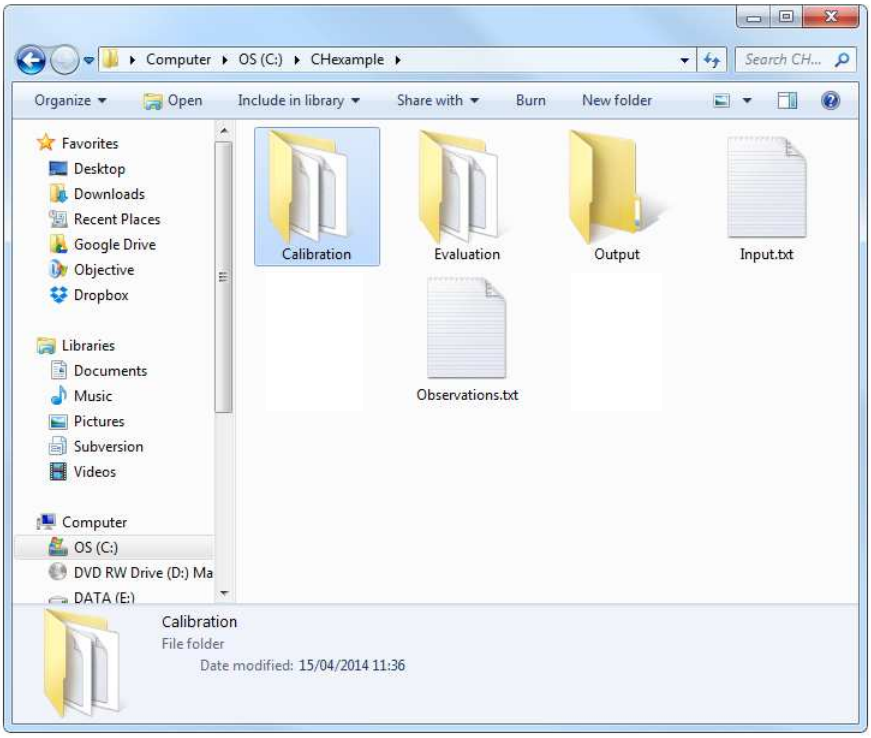

Figure 5.1 Folder structure of AquiMod.

5.2 INPUT FILES

5.2.1 Observations.txt

Before running AquiMod, the user must specify four observation time-series as shown in Table 5.1. These time-series can be summarised as follows:

- **Climate (rainfall and PET)**

A continuous time-series of rainfall and PET data is required to drive the model, specified in units of mm d^{-1}.

- **Groundwater levels**

At least one time-stamped measurement of groundwater level is required specified in units of metres above a datum. AquiMod uses these data to calculate the specified objective function. Where measurements are not available, a -9999 value should be entered.

- **Abstraction rates**

A continuous abstraction rate time-series specified in units of $m^3 d^{-1}$ is required. This is subtracted from the saturated zone component during simulation.

The number of observations must also be input on line 2. In the example shown in Table 5.1, a total of 540 time-steps are specified which run from January 1961.

Table 5.1 Example Observations.txt file.

Line number	File text							Description
1	NUMBER OF OBSERVATIONS							Comment Line
2	540							Number of time-steps for simulation
3	DAY	MONTH	YEAR	RAIN	PET	GWL	ABS	Headers for columns
4	31	1	1961	4.8	0.42	70.7	0.0	[day, month, year, rain (mm d^{-1}), PET (mm d^{-1}), groundwater level (m), groundwater abstraction rate ($m^3 d^{-1}$)]
5	28	2	1961	3.1	0.54	67.6	0.0	.
6	31	3	1961	0.07	1.1	59.3	0.0	.
.	.							.
.	.							.

The Observations.txt file can also be used to specify a number of other conditions including:

5.2.1.1 MODEL TIME-STEP

The model time-step is defined by the length of time between each time-stamp in the Observations.txt file. The minimum time-step is one day and the time-step length can vary throughout the simulation sequence. Note that in Table 5.1, the model has been configured to run on a monthly time-step, producing groundwater level simulations at the end of each month.

5.2.1.2 INITIAL CONDITIONS

AquiMod assumes a dry soil and unsaturated zone initially. The saturated zone is always initialised at the first time-step where an observed groundwater level measurement is available in Observations.txt. If this is not the first time-step, as well as initialising the model at the first groundwater level observation, AquiMod also uses the mean of all available groundwater level data in Observations.txt to initialise the model at the first time-step. In the example, the first time-step has a groundwater level measurement of 70.7 m, and as such this is used to initialise the saturated zone component.

5.2.1.3 IMPOSED GROUNDWATER LEVELS

As well as initialising the model with the observed groundwater levels, it is also possible to impose observed groundwater levels mid-simulation. By doing so, the model discards the simulated level for that time-step and uses the observed level instead. This can be done at one or more time-steps by placing an asterisk at the end of the corresponding row(s) in Observations.txt (Table 5.2).

Table 5.2 Imposing groundwater levels in the Observations.txt file.

Line number	File text								Description
1	NUMBER OF OBSERVATIONS								
2	540								
3	DAY	MONTH	YEAR	RAIN	PET	GWL	ABS		
4	31	1	1961	4.8	0.42	70.7	0.0		
5	28	2	1961	3.1	0.54	67.6	0.0	*	Here the simulated groundwater level will be discarded and set to the observed level
6	31	3	1961	0.07	1.1	59.3	0.0		.
.	.								.
.	.								.

5.2.2 Input.txt

The Input.txt file is where the user can specify a number of different options, each indicated by a corresponding header line (Table 5.3). These are detailed as follows:

- **Component IDs**

The ID numbers for the desired soil, unsaturated and saturated zone components as indicated in the Tables in section 3. For example, in Table 5.3 all have been set to 1 which indicates that the FAO, Weibull and Q3K3S1 components are to be used.

- **Simulation mode**

Here, the choice of either calibration ('c') or evaluation ('e') mode is specified.

- **Number of runs**

The number of runs can range from 1 to approximately 10^7 (the maximum in calibration mode is dependent on available computer memory).

- **Objective function**

Here, the objective function used to evaluate the model simulations against the observed levels in Observations.txt is specified.

- **Spin-up period**

Due to the fact that the soil and unsaturated zone components are initiated without any water in them, there is an initial wetting-up period, or spin-up period where AquiMod may not be able to simulate the groundwater level time-series adequately which can result in poor optimization of the model parameters when running in calibration mode. To prevent this, the length of this period should be specified as a number of time-steps. AquiMod will then ignore this portion of the simulation when calculating the chosen objective function.

The length of this period is likely to depend on the choice of model structure and parameters. Past experience has shown that the unsaturated zone component often has the longest "memory" of the three components in AquiMod. For example, when using the Weibull unsaturated zone component, the n parameter, which defines the number of time-steps over which recharge is spread, can also be used to define the spin-up period (see section 6.1 for further information on defining the spin-up period).

- **Acceptable model threshold**

This option is only applicable when running AquiMod in the Monte Carlo calibration mode. It defines the objective function threshold that must be reached, for the parameter set of the simulation to be stored and output.

- **Maximum number of acceptable models**

This option is only applicable when running AquiMod in the Monte Carlo calibration mode. It defines the maximum number of parameter sets that exceed the acceptable threshold that will be output. Note that AquiMod uses the quick sort algorithm to sort the Monte Carlo runs by objective function. Simulation time may increase if large numbers of acceptable parameter sets are stored.

- **Write model output files**

Here, the user can specify if they wish output files to be written for each model component. When running in calibration mode, a single file is output for each component. In evaluation mode, a separate file is output for each model component and model run which may slow down the overall model run-time.

Table 5.3 Example Input.txt file.

Line number	File text	Description
1	Component IDs	Comment Line
2	1 1 1	Module component selection [Soil, Unsat., Sat.] (integers)
3		Blank
4	Simulation mode	Comment Line
5	e	Simulation mode
		c = calibration
		e = evaluation
6		Blank
7	Number of runs	Comment Line
8	1	Number of model runs (for calibration and evaluation modes)
		1 to ~10^7 (integer)
9		Blank
10	Objective function	Comment Line
11	1	Objective function ID (integer)
12		Blank
13	Spin-up period	Comment Line
14	6	Spin up period over which objective function will not be calculated.
		number of time-steps (integer)
15		Blank
16	Acceptable model threshold (calibration only)	Comment Line
17	0.9	Objective function which must be reached for results to be output (float)
18		Blank
19	Maximum number of acceptable models (calibration only)	Comment Line
20	1	Maximum number of acceptable models output from calibration mode (integer)
21		Blank
22	Write model output files	Comment Line
23	Y Y Y	Switch for writing output files [Soil, Unsat., Sat.]
		Y = yes write output file
		N = no do not write output file

5.2.3 Calibration input files

When running in calibration mode, a separate input file for each module component must be configured in the Calibration folder. These files specify the range of values from which the Monte Carlo parameter sets are randomly sampled (see Appendix 1 for a list of recommended ranges). All files have the same naming convention: *_calib.txt where the asterisk should be replaced by the component name. An example of the FAO_calib.txt calibration input file is given in Table 5.4. Note the general structure: header lines followed by two numerical values which specify the maximum and the minimum of the range of values to be sampled randomly. Also note that parameters can be fixed simply by specifying the same minimum and maximum values, as has been done for the field capacity parameter.

Note that template files for all module components can be downloaded from the AquiMod website.

Table 5.4 Example of the FAO_calib.txt calibration input file format. The field capacity (line 2) is fixed while the root depth (line 8) will change for each calibration run.

Line number	File text	Description
1	Field Capacity(-)	Comment Line
2	0.31 0.31	Minimum and maximum value
3		Blank
4	Wilting Point(-)	Comment Line
5	0.1 0.2	Minimum and maximum value
6		Blank
7	Root Depth(mm)	Comment Line
8	100 3000	Minimum and maximum value
9		Blank
10	Depletion Factor(-)	Comment Line
11	0.01 0.99	Minimum and maximum value
12		Blank
13	Baseflow index(-)	Comment Line
14	0.7 0.9	Minimum and maximum value

5.2.4 Evaluation input files

In evaluation mode, AquiMod requires the user to specify one or more parameter sets using input text files for each module component. These files must be located in the Evaluation folder and they follow a standard naming convention: *_eval.txt where the asterisk should be replaced by the component name. Table 5.5 provides an example of the FAO_eval.txt file. Here only a single parameter set is defined, but multiple parameter sets can be included on separate lines (e.g. see Section 6.2).

Table 5.5 Example of FAO_eval.txt file.

Line number	**File text**						**Description**
1	FieldCapacity(-)	WiltingPoint(-)	MaxRootDepth(mm)	DepletionFactor(-)	BaseflowIndex(-)		Header Line
2	0.31	0.15	2000.0	0.6	0.85		Parameter values

5.3 OUTPUT FILES

After executing the AquiMod software, a series of output files will be generated in the Output folder (the number of files generated depends on the user specifications in Input.txt). All output files use the '.out' file extension.

5.3.1 Calibration output files

Assuming that the output file switches in the input.txt file have all been set to 'Y', AquiMod will produce a single output file for each module component selected for a calibration run. These files follow the naming convention *_calib.out where the asterisk is replaced by the component name. An example Weibull_calib.out file is shown in Table 5.6. Within these files, the parameter sets that resulted in a simulation that met acceptable model threshold (as defined in input.txt) are listed.

Note that the file structure is identical to the evaluation input files. This allows for easy transfer between calibration and evaluation modes (see Section 6.2).

Table 5.6 Example of FAO_calib.out file.

Line number	File text				Description
1	k(-)	lambda(-)		n(timesteps)	Header Line
2	2.78	2.43	6		Parameter values
3	4.43	2.10	6		.
4	6.49	1.64	6		.
5	3.12	2.06	6		.
.	.				.
.	.				.

In conjunction with the module component output files, a fit_calib.out file is also produced (see example in Table 5.7) which lists the corresponding objective function scores of the acceptable parameter sets obtained.

Table 5.7 Example of fit_calib.out file produced by AquiMod using the NSE objective function.

Line number	File text	Description
1	ObjectiveFunction	Header Line
2	0.913	Objective function score
3	0.912	.
4	0.908	.
5	0.907	.
.	.	.
.	.	.

5.3.2 Evaluation output files

Assuming that the output file switches in the input.txt file have all been set to 'Y', AquiMod will produce a time-series output files for each parameter set specified in the *_eval.txt files and each module component selected for a given evaluation run. These files follow the naming convention

[1]_TimeSeries[2].out where *[1] is the component name and *[2] is the model run number. An example of the Q3K3S1 output file for parameter set 1 is shown in Table 5.8. Note that here the output variables include the simulated discharges from the three outlets and the groundwater level time-series. For more information on the output variables produced for each module component see Appendix 2.

A corresponding fit_eval.out file is also produced which returns the objective function score for each parameter set. The structure of this file is identical to that for a calibration run (Table 5.6).

Table 5.8 Example of Q3K3S1_TimeSeries1.out from an evaluation run.

Line number	File text							Description
1	Day	Month	Year	Q3(m3/d)	Q2(m3/d)	Q1(m3/d)	GWL(m)	Header Line
2	31	1	1961	0 0	0 70.665			Variable values
3	28	2	1961	4.82748	5.21203	0.248902	61.1048	.
4	31	3	1961	0.893412	4.06564	0.219899	55.6219	.
5	30	4	1961	0.0516189	3.40817	0.203265	53.9034	.
6	31	5	1961	4.61944e-006	3.20209	0.198052	50.2362	.
.	.							.
.	.							.

6 Tutorials

This section provides a series of step-by-step tutorials that can be used to familiarise yourself with the AquiMod software. All of the examples shown use the model in the CHexample folder. If you do not have this already, follow the instructions in section 2.

6.1 HOW TO PERFORM A CALIBRATION RUN

This tutorial provides instructions to calibrate an AquiMod model for an observation borehole catchment in the United Kingdom. You will configure the Observations.txt and Input.txt files and learn about the calibration input files. You will then run a Monte Carlo calibration procedure and examine the model outputs.

6.1.1 The Chilgrove House observation borehole

The Chilgrove House observation borehole is located in the Cretaceous Chalk aquifer in the south of the United Kingdom (Figure 6.1). It has groundwater level records from 1836 and is one of the longest groundwater level time-series in the world. Situated in the unconfined Seaford Chalk formation, the hydrograph displays a typical sinusoidal response generated by the seasonal recharge signal typical of unconfined aquifers in the UK. More information on the Chilgrove House observation borehole can be found on the British Geological Survey web-site at http://www.bgs.ac.uk/research/groundwater/datainfo/levels/sites/ChilgroveHouse.html. In this tutorial, you will focus on a 45-year time-series of groundwater level data between January 1961 and December 2005 over which reliable rainfall and PET estimates are also available (Figure 6.2).

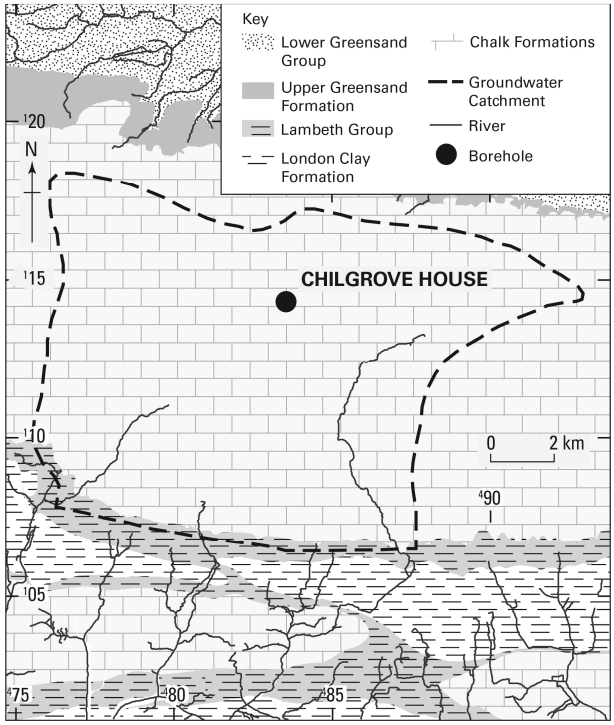

Figure 6.1 Location of Chilgrove House observation borehole along with geological setting and nearby river network.

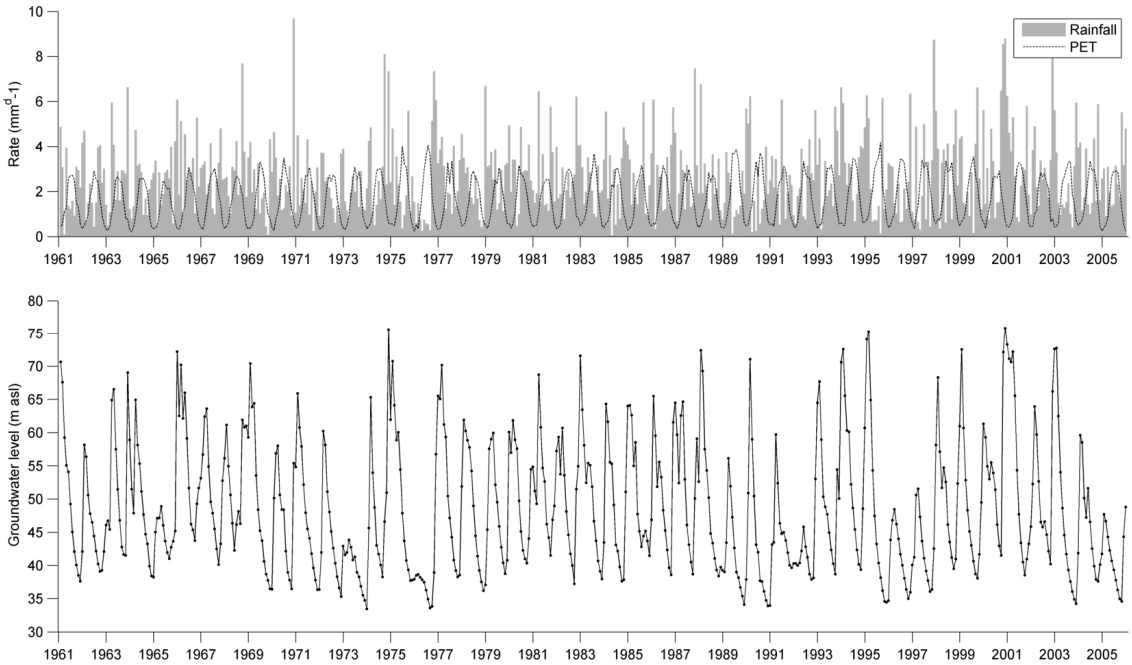

Figure 6.2 Observed rainfall, PET (top) and groundwater level data (bottom) for the Chilgrove House observation borehole catchment.

6.1.2 Observations.txt

First you will calibrate the model against the first half of observed groundwater data between January 1961 and June 1983. This half of the data can be found in ObsCalib.txt. **Copy and paste this in Observations.txt**. Note that there is no significant groundwater abstraction in the catchment, and as such these rates have been set to zero. Also note that the model will run on a monthly time-step.

6.1.3 Input.txt

Next, you will configure the Input.txt file as shown in Figure 6.3. Open this file in a text editor. Going through each option in order:

- **Component IDs** – you will use the FAO, Weibull and Q3K3S1 module components so these should all be set to 1.
- **Simulation mode** –this should be set to 'c' to run in calibration mode.
- **Number of runs** – for this tutorial you will run the model 100,000 times in order to find the most efficient parameter sets.
- **Objective function** – you will use the NSE as the measure of model fit and so this should be set to 1.
- **Spin-up period** – a spin-up period of 6 time-steps (months) is sufficient for this observation borehole catchment.
- **Acceptable model threshold** – deciding upon a suitable value for this will depend on the type of application and personal preferences. For this tutorial, an arbitrary value of 0.8 will be used.
- **Maximum number of acceptable models** – again, defining this value is likely to depend on the proposed application. For this tutorial, you will only consider the most efficient 1000 models (assuming 1000 exceed the acceptable model threshold).
- **Write model output files** – in calibration mode, the output files will contain the parameter sets of the most efficient Monte Carlo simulations. You will need this information later on, so set all of these to 'Y'.

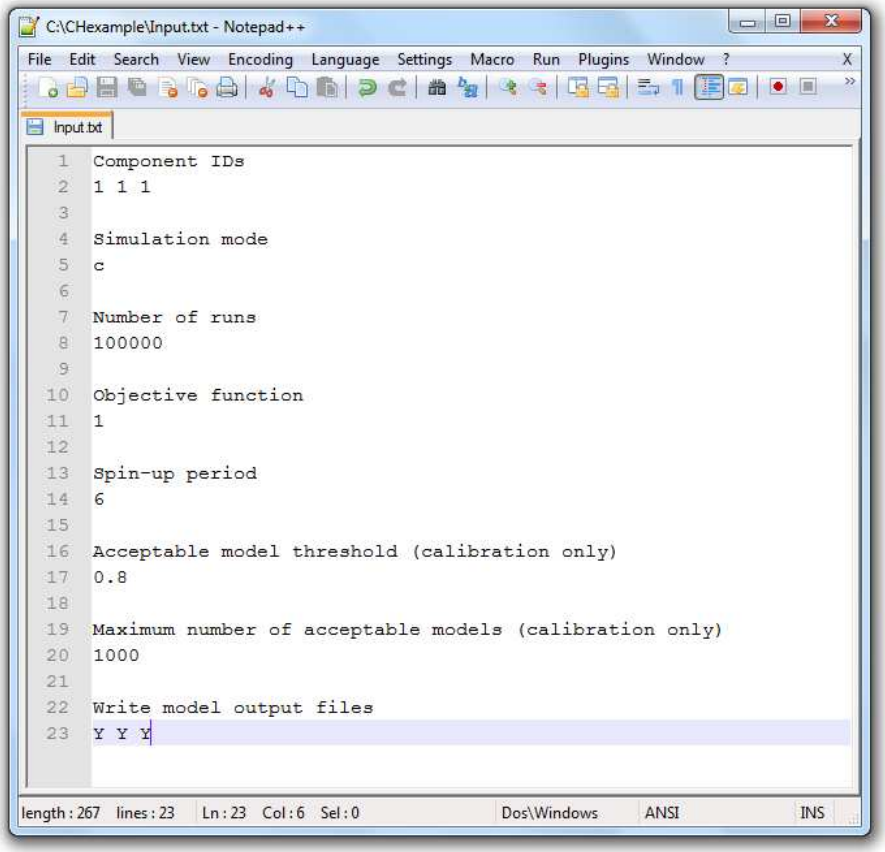

Figure 6.3 Configured Input.txt file for the Chilgrove House calibration run.

6.1.4 Calibration input files

For this example, the calibration input files have been pre-configured so that a total of 8 of the 16 parameters will be calibrated, while the remainder are fixed. This was determined based on the availability of catchment data.

Open the FAO_calib.txt file located in the Calibration folder. The field capacity, wilting point and baseflow index parameters have been fixed based on known catchment information obtained from a soil database of the United Kingdom (Boorman et al., 1995) while the maximum root depth and depletion factor are to be randomly sampled between specified ranges.

Next, **open the Weibull_calib.txt file**. The Weibull lambda and n parameters have been determined by analysing the relationship between rainfall and groundwater levels. The lambda parameter controls the location of the peak of the Weibull distribution, or in other words the peak recharge response to rainfall and subsequent soil drainage. As such, a cross-correlation analysis has been performed between monthly rainfall and groundwater levels (Figure 6.4) that shows a peak correlation at a 1 month lag. Accordingly, the lambda range has been set from 1 – 2.5. The n parameter has been set to 6 as this is the longest lag that shows a significant correlation (also note that this was used to define the spin-up period in Input.txt). The k parameter range has been set to 1-7 which is a typical range for this distribution parameter.

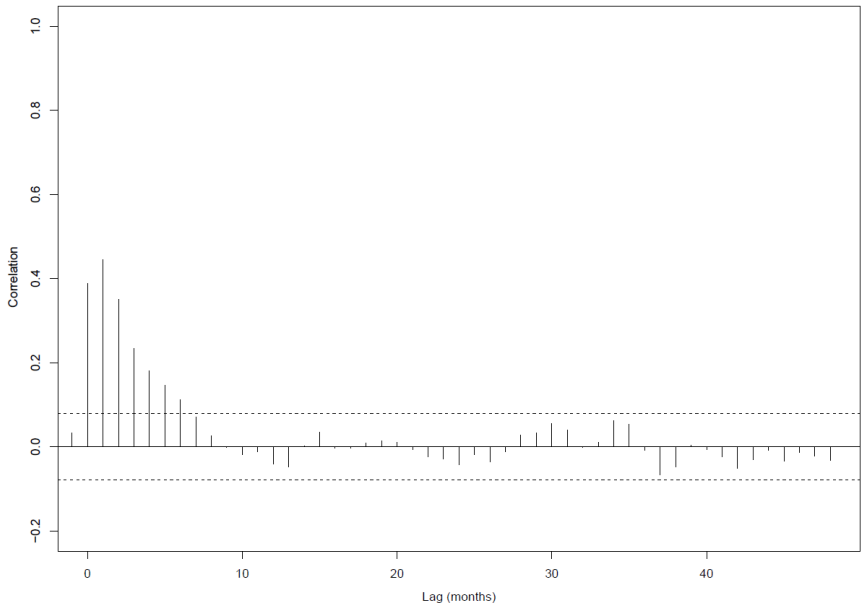

Figure 6.4 Cross-correlations between rainfall and de-seasonalised groundwater levels.

Finally, **open Q3K3S1_calib.txt**. The aquifer length has been fixed to 3000 m which is the approximate length between the borehole and the nearest river in the catchment where the groundwater discharges. The bottom elevation of the aquifer has been set based on the known geometry of the Chalk aquifer in this catchment. The second layer outlet elevation has also been set. The top layer elevation has been kept as a calibration parameter and is free to fluctuate between ground level elevation and the minimum groundwater level on record (i.e. within the zone of fluctuation). The specific yield and hydraulic conductivity ranges have been set based on known Chalk properties. In this case, the conductivities have been set to decrease with depth as this is a common characteristic of the Chalk aquifer. Due to the fact that some of the conductivity ranges between layers overlap, the alpha parameter has been set to 1 to ensure that the conductivity decreases with depth.

6.1.5 Running AquiMod in calibration mode

Having configured all of the required input files, AquiMod is now ready to run as shown in section 2.2. **Run AquiMod in the command prompt.** Notice a slight difference in the output messages for this run in comparison to the initial evaluation run conducted in section 2.2 (Figure 6.5). The first message states that the model is running 100,000 times. The second states that it is extracting the best models. Generally this is instantaneous, but when storing large numbers of parameter sets it can become the bottleneck in the overall simulation run-time. Finally it writes the output files to the Output folder and then states the total run-time.

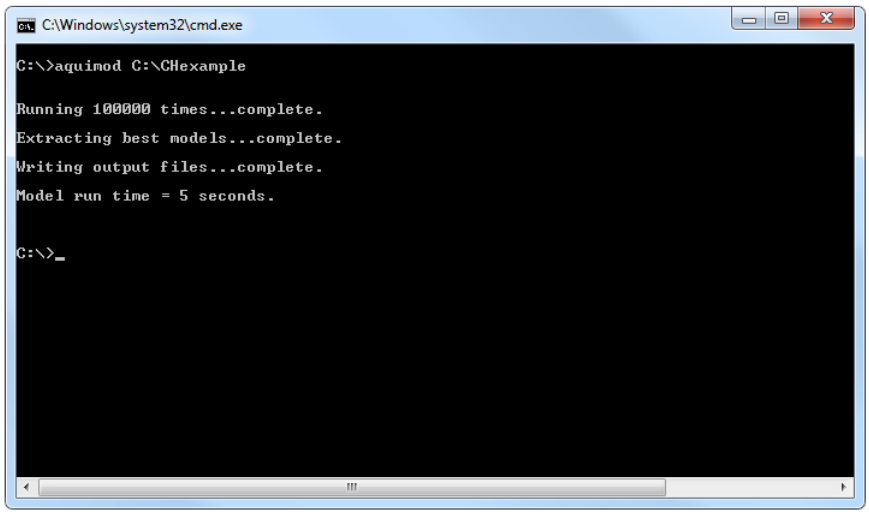

Figure 6.5 Command prompt view when running AquiMod in calibration mode.

6.1.6 Output files

Navigate to the Output folder. AquiMod should have produced a fit_calib.out file as well as a *_calib.out file for each of the three module components. Open the fit_calib.out file to check if any acceptable models have been obtained. The file should be filled with up to 1000 NSE scores. You can use the fit_calib.out file in conjunction with the *_calib.out module component files to assess the sensitivity of the parameters. For example, in Figure 6.6 two dotty plots have been drawn in MATLAB which indicate that the S parameter shows more sensitivity than the K3 parameter.

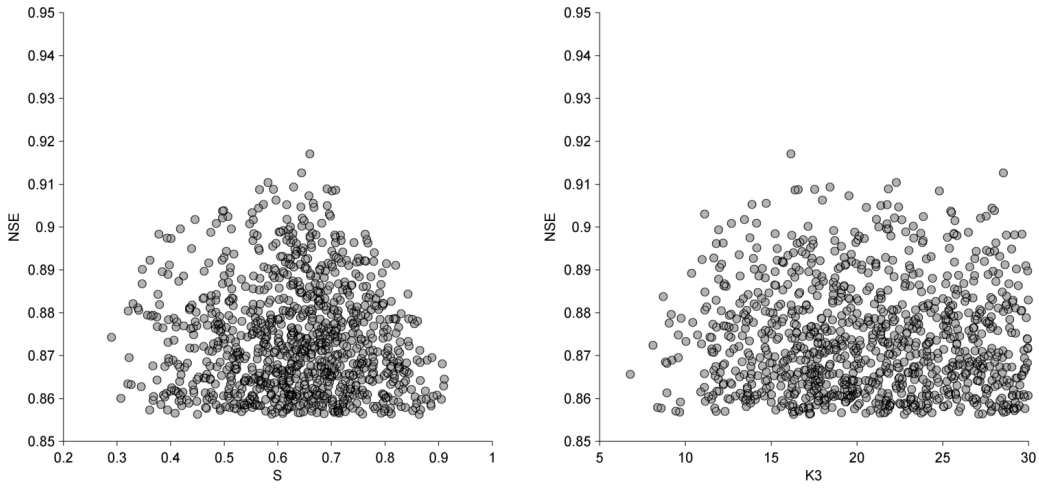

Figure 6.6 Dotty plots to assess sensitivity of S (%) (left) and K3 (m d^{-1}) (right) parameters from the Q3K3S1 saturated zone component. Plots contain 1000 acceptable models obtained from the calibration run.

If the fit_calib.out file is empty, that means no acceptable models have been obtained. In this case, you may wish to reconsider the criteria for accepting a model, increase the number of runs, adjust the parameter calibration ranges or experiment with different model structures.

6.2 HOW TO PERFORM AN EVALUATION RUN

This tutorial provides guidance on how to use AquiMod in evaluation mode. Here AquiMod does not employ the Monte Carlo parameter sampling. Instead, you are required to specify the parameters. As such, in evaluation mode, AquiMod does not output any information on model parameters, but instead generates the simulated time-series for the defined parameter sets. In this sense it allows you to evaluate specific model structures and parameter sets by visually comparing the observed and simulated time-series.

In this tutorial you will evaluate your newly derived parameter sets from the previous section against all of the available data between January 1961 and December 2005.

6.2.1 Observations.txt

First, you need to specify the observed sequence in the Observations.txt file. This data can be found in ObsEval.txt. Simply **copy and paste** this into Observations.txt. Note that as before, we are still running the model on a monthly time-step with no abstraction.

6.2.2 Input.txt

Next, you will configure Input.txt. **Open Input.txt in a text editor**. Going through each option in order:

- **Component IDs** – this should remain the same as you will use the same module components.
- **Simulation mode** – set this to ‘e’ to run AquiMod in evaluation mode.
- **Number of runs** – Set this to the number of acceptable parameter sets that were obtained from the previous tutorial.
- **Objective function** – this should remain the same.
- **Spin-up period** – this should remain the same.
- **Acceptable model threshold** – this option is not used in evaluation mode.
- **Maximum number of acceptable models** – this option is not used in evaluation mode.
- **Write model output files** – in evaluation mode, the output files will contain the time-series simulations for the acceptable models. In this tutorial you will only assess the groundwater level simulations, so set the first two to ‘N’ and the last one to ‘Y’.

Figure 6.7 shows the completed Input.txt file for this exercise.

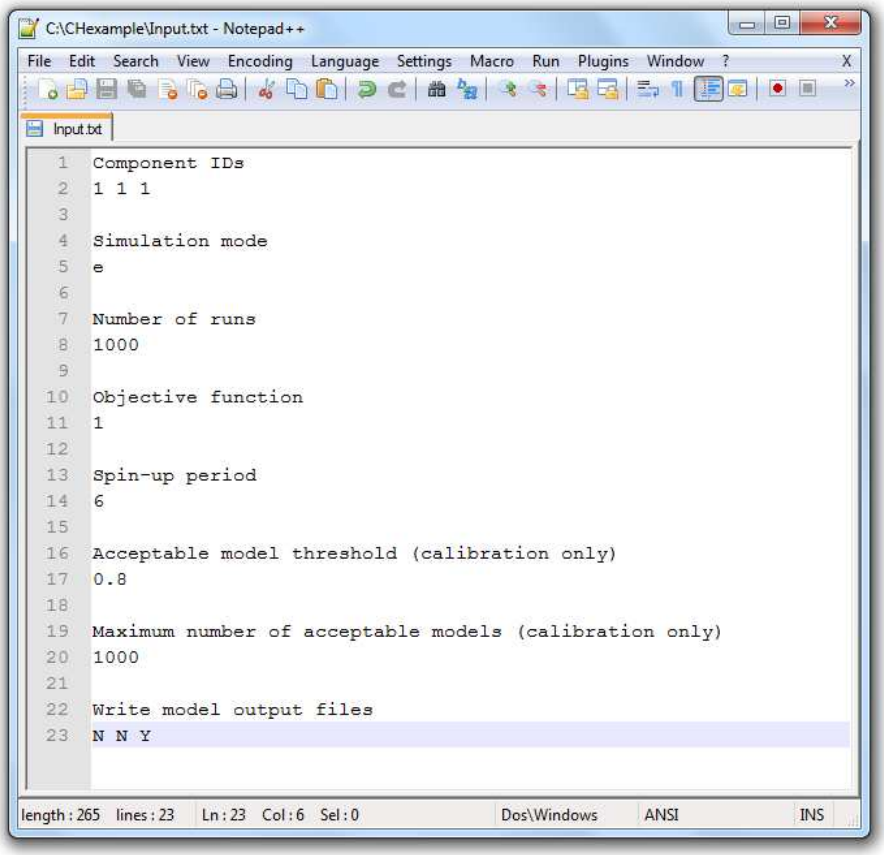

Figure 6.7 Configured Input.txt file for the Chilgrove House evaluation run.

6.2.3 Evaluation input files

The file structure of the *_eval.txt input files is exactly the same as the output files from the calibration mode. Since you will evaluate the calibrated parameter sets, these files can simply be moved to the Evaluation folder and renamed accordingly. For example Output\Q3K3S1_calib.out **should be moved and renamed to** Evaluation\Q3K3S1_eval.txt.

6.2.4 Running AquiMod in evaluation mode

Having configured all of the required input files, AquiMod is now ready to run as shown in section 2.2. **Run AquiMod in the command prompt**. This should return similar messages as the calibration run (Figure 6.8).

Note that the runtime is longer for these evaluation runs, even though far fewer runs have been performed than the 100,000 in the previous tutorial. This is because AquiMod has to write a time-series file for each run. As such, when performing large numbers of evaluation runs and outputting the results, runtime can increase considerably.

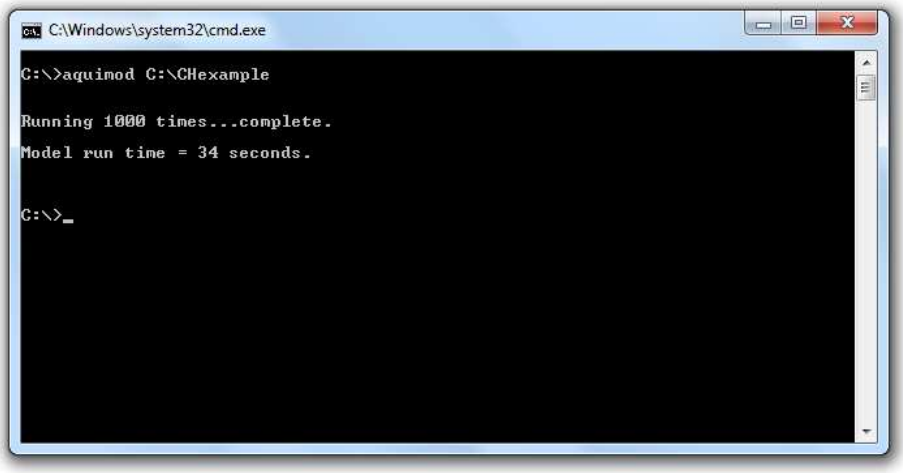

Figure 6.8 Command prompt view when running AquiMod in evaluation mode.

6.2.5 Output files

After running AquiMod in evaluation mode, it should have produced a fit_eval.out file in the Output folder as well as time-series files for each parameter set for the Q3K3S1 module component. Individual time-series can easily be plotted in applications such as Microsoft Excel. However, plotting the full range of simulations is often faster using a scripting language. Figure 6.9 has been produced using MATLAB and shows the 90% bands of all the simulations in blue (calibration sequence) and red (evaluation sequence) against the observations (black dots).

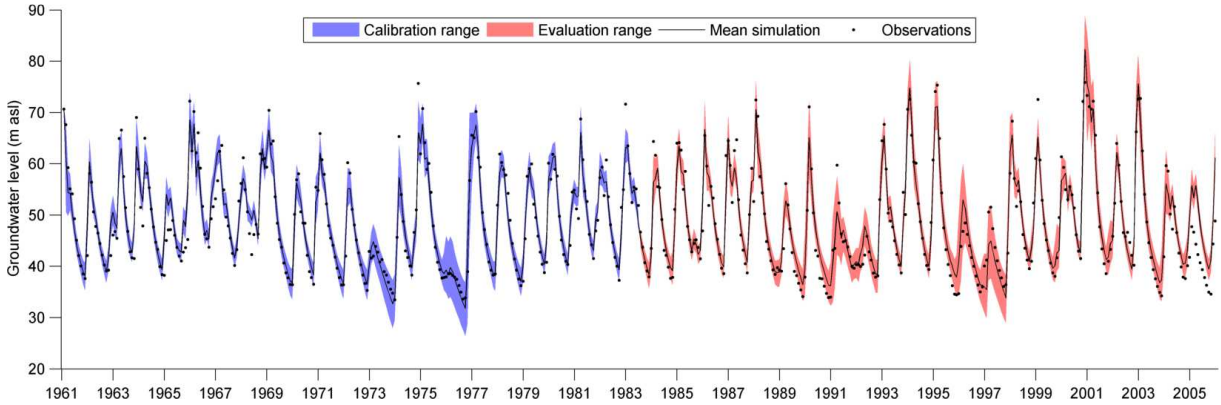

Figure 6.9 Range of simulations shown in blue (calibration sequence) and red (evaluation sequence) with the mean simulation (solid black) and observations (black dots).

6.3 DEACTIVATING MODULES AND USING OTHER COMPONENTS

You may select any combination of the available module components when using AquiMod. You may also deactivate modules entirely using the ID '0' in Input.txt if you only wish to consider part of the hydrological system. This may be useful for example if a boundary condition flux is known and therefore does not need to be simulated, or if part of the hydrological system is not deemed to be important for a particular application.

If the soil zone is deactivated, evapotranspiration is assumed to be zero and rainfall passes directly to the unsaturated zone as soil drainage. If the unsaturated zone is deactivated, soil drainage is allowed to pass instantaneously the saturated zone. If both the soil and unsaturated zone are deactivated, the rainfall input essentially becomes a recharge input to the saturated

zone. If the saturated zone is deactivated, groundwater recharge discharges instantaneously out of the model domain.

As a final exercise, experiment with deactivating different modules in the AquiMod structure. You should find for the Chilgrove House observation borehole catchment that efficient simulations of groundwater levels can still be reproduced without the inclusion of the unsaturated zone component.

You may also wish to experiment with using other components. This can be done simply by changing the options in Input.txt and the associated input files. For this, it is recommended to use the template files available on the AquiMod website.

Appendix 1

List of component parameters and recommend range of values to be used.

SOIL ZONE COMPONENT PARAMETERS

FAO

Parameter (units)	Description	Recommend Range (variable type)
BFI (-)	Catchment baseflow index	0 – 1 (float)
FC (-)	Field capacity of the soil	0 – 1 (float)
WP (-)	Wilting point of the soil	0 – 1 (float)
Zr (mm)	Maximum rooting depth of catchment vegetation	100 – 3000 (float)
p (-)	Depletion factor of catchment vegetation	0 – 1 (float)

UNSATURATED ZONE COMPONENT PARAMETERS

Weibull

Parameter (units)	Description	Recommend Range (variable type)
n (-)	Maximum number of time-steps taken for soil drainage to reach the groundwater	>0 (integer)
k (-)	Weibull shape parameter	1 – 7 (float)
λ (-)	Weibull scale parameter	>0 (float)

SATURATED ZONE COMPONENT PARAMETERS

Q3K3S1

Parameter (units)	Description	Recommend Range (variable type)
Δx (m)	Catchment length	>0 (float)
K_3 (m d^{-1})	Top layer hydraulic conductivity	10^{-5} - 10^{3} (float)
K_2 (m d^{-1})	Middle layer hydraulic conductivity	10^{-5} - 10^{3} (float)
K_1 (m d^{-1})	Bottom layer hydraulic conductivity	10^{-5} - 10^{3} (float)
S (%)	Aquifer storage coefficient	0 – 1 (float)
z_3 (m asl)	Top outlet elevation	-∞ - ∞ (float)
z_2 (m asl)	Middle outlet elevation	-∞ - ∞ (float)
z_1 (m asl)	Bottom outlet elevation	-∞ - ∞ (float)
α (-)	Forces the hydraulic conductivity to increase with elevation when set to 1	0,1 (bool)

Appendix 2

List of output variables produced in time-series files for each module component.

SOIL ZONE COMPONENT OUTPUT VARIABLES

FAO

Variable (units)	Description
Runoff (mm d^{-1})	Surface runoff
AET (mm d^{-1})	Actual evapotranspiration from soil
SMD (mm)	Soil moisture deficit
Soil Drainage (mm d^{-1})	Soil drainage to unsaturated zone

UNSATURATED ZONE COMPONENT OUTPUT VARIABLES

Weibull

Variable (units)	Description
Recharge (mm d^{-1})	Recharge to the saturated zone

SATURATED ZONE COMPONENT OUTPUT VARIABLES

Q3K3S1

Variable (units)	Description
Q_3 (m^3 d^{-1})	Groundwater discharge from top aquifer layer
Q_2 (m^3 d^{-1})	Groundwater discharge from middle aquifer layer
Q_1 (m^3 d^{-1})	Groundwater discharge from bottom aquifer layer
GWL (m above datum)	Groundwater level

Q2K2S1

Variable (units)	Description
Q_2 (m^3 d^{-1})	Groundwater discharge from the top aquifer layer
Q_1 (m^3 d^{-1})	Groundwater discharge from bottom aquifer layer
GWL (m above datum)	Groundwater level

Q1K1S1

Variable (units)	Description
Q_1 (m^3 d^{-1})	Groundwater discharge
GWL (m above datum)	Groundwater level

Q1T1S1

Variable (units)	Description
Q_1 (m^3 d^{-1})	Groundwater discharge
GWL (m above datum)	Groundwater level

VKD

Variable (units)	Description
Q_1 (m^3 d^{-1})	Groundwater discharge
GWL (m above datum)	Groundwater level

References

The British Geological Survey holds most of the references listed below, and copies may be obtained via the library service subject to copyright legislation (contact libuser@bgs.ac.uk for details). The library catalogue is available at: http://geolib.bgs.ac.uk.

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